Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Perovskite Al-$SrTiO_3$ semiconductor electrolyte with superionic conduction in ceramic fuel cell

M.A.K. Yousaf Shah[1], Yuzheng Lu [2*], Naveed Mushtaq[1], Muhammad Yousaf[1], Sajid Rauf[3], Muhammad Imran Asghar[4*], Peter D Lund[4], Bin Zhu[1*]

[1]*School of Electronic Engineering, Nanjing Xiao Zhuang University, 211171 Nanjing, China.*

[2]*Jiangsu Provincial Key Laboratory of Solar Energy Science and Technology/Energy Storage joint Research Center, School of Energy and Environment, Southeast University, No.2 Si Pai Lou, Nanjing 210096, China.*

[3]*College of Electronics and Information Engineering, Shenzhen University, Guangdong Province, 518000, China.*

[4]*New Energy Technologies Group, Department of Applied Physics, Aalto University School of Science, P. O. Box 15100, FI-00076 Aalto, Espoo, Finland.*

Corresponding author, Bin Zhu

Email address: zhu-bin@seu.edu.cn

Corresponding author, Yuzheng Lu

Email address: mrluyuzheng@163.com

Corresponding author, Muhammad Imran Asghar

Email address: imran.asghar@aalto.fi

Fig.1 shows the XRD (x-ray diffraction) pattern of Al: STO powder before and after testing. The below Fig confirms to obtain pure perovskite structure before but after performance structure

remains same, but it got some peaks of $LiCO_3$, NiO and Ni which signifying that NCAL got reduced into LiOH, NiO, Ni and formed $LiCO_3$ as demonstrated in XRD pattern. So, XRD confirms the formation of the $LiCO_3$ layer after testing as seen in below Fig.1 [1,2].

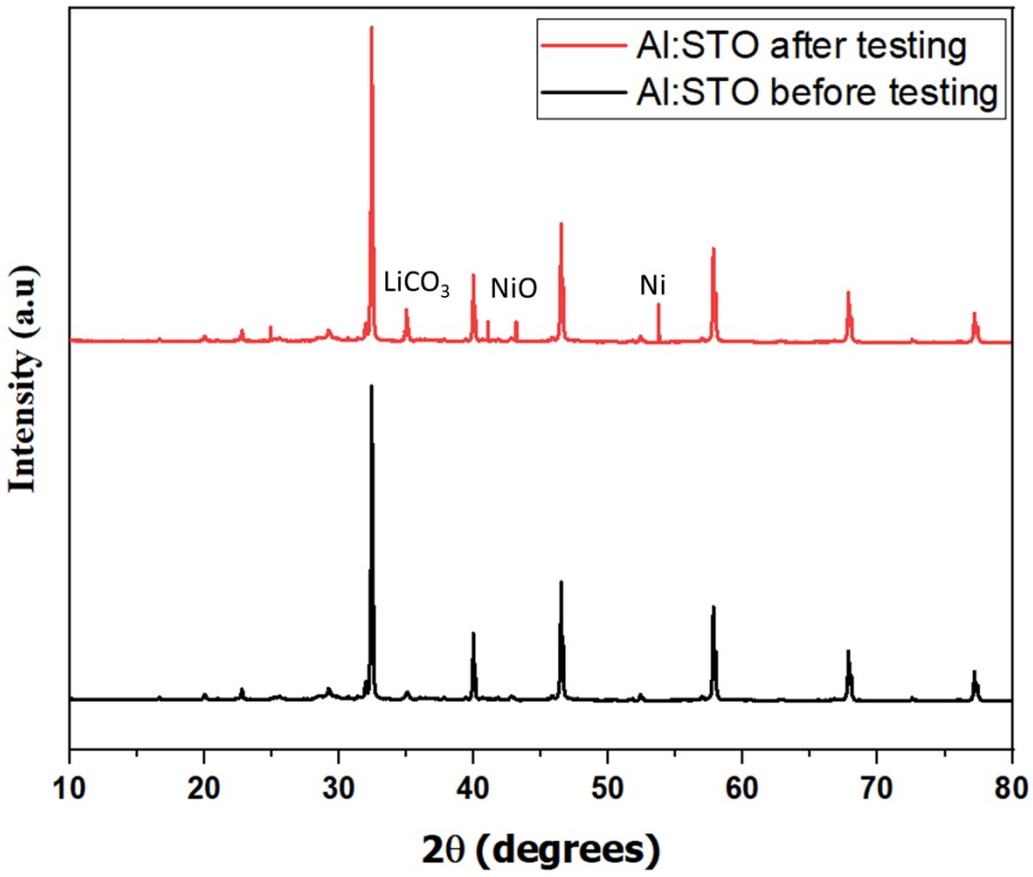

Fig.1 XRD pattern of Al: STO before and after testing

Fig.2 (a, b) shows the SEM (scanning electron microscopy) images of STO and Al: STO. The SEM images are suggesting that all particles are uniformly and coherently distributed and well connected with each other leading to the proper way of charge transportation. Also, by doping the density of particles been enhanced also the size of particles got reduced which causes to enhance the surface area to create more active site for the transportation of charges. Fig.2(c) shows the HR-TEM image of Al: STO before testing which clearly suggesting that there is no amorous phase being noticed [1,2].

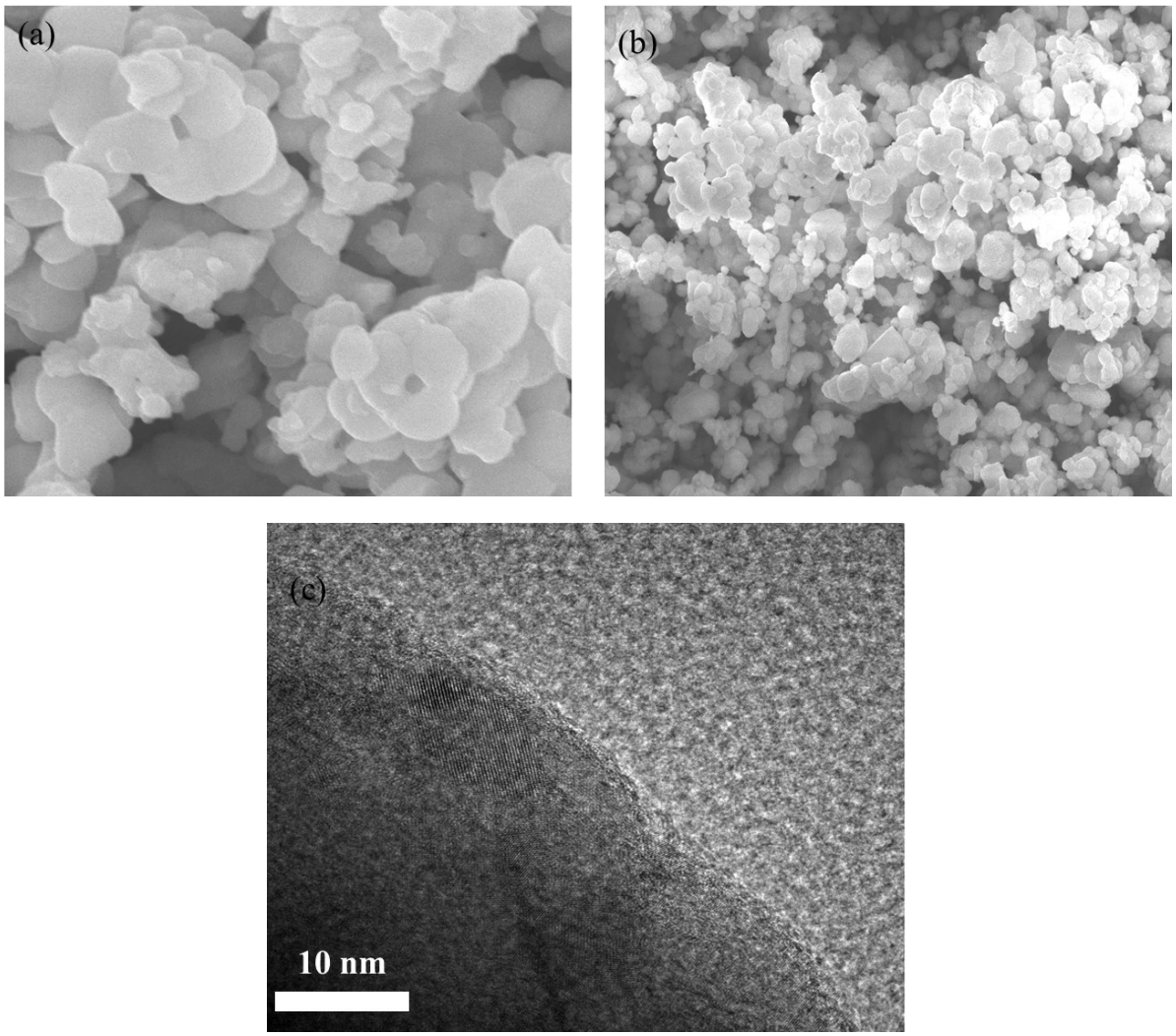

Fig. 2 (a, b) Scanning electron microscopy images of STO and AL: STO at 1 um magnification scale while (c) shows the HR-TEM image of Al: STO before testing

Fig.3 shows the dc four-probes ionic conductivity of synthesized electrolyte Al: STO at different operational temperatures 520-420 ^{o}C.

Table 1: The EIS fitted data of the $SrTiO_{3-\delta}$ electrolyte layer cell materials at different temperatures of 520-420 °C.

T	L	R_o	R_1	Q_1	n	C_1	R_2	Q_2	n	C_2
520 °C	1.516E-7	0.322	0.06	0.7726	0.3	0.0006	0.2429	1.055	0.6	0.4261
470 °C	1.583E-7	0.44	0.08	0.7161	0.2	$5E^{-6}$	0.38	0.6131	0.7	0.3325
420 °C	1.77E-7	0.64	0.12	0.373	0.6	0.057	0.6	0.3696	0.2	0.0008

Table 2: The EIS fitted data of the Al: $SrTiO_{3-\delta}$ electrolyte cell materials at different temperatures of 520-420 °C.

T	L	R_o	R_1	Q_1	n	C_1	R_2	Q_2	n	C_2
520 °C	8.374E-8	0.18	0.045	1.558	0.30	0.0031	0.23	5.619	0.96	5.6769
470 °C	6.713E-8	0.20	0.06	1.156	0.28	0.0014	0.36	5.068	0.8	5.8900
420 °C	9.185E-8	0.29	0.073	1.232	0.65	0.3437	0.57	0.955	0.27	0.1848

The XPS analysis was carried out to evaluate the surface chemical and oxidation state of STO and Al: STO, and to observe the oxygen vacancies in the doped STO. Fig 3 shows the full XPS spectra

of STO and Al: STO with different orbitals 3s, 3p, 3d, 3d, 2p, and 1s, respectively. It is found that the characteristic peaks of Al: STO are shifting toward the lower binding energy, which usually signifies the decrease in valence state, leading to the release of oxygen ions [3,4]

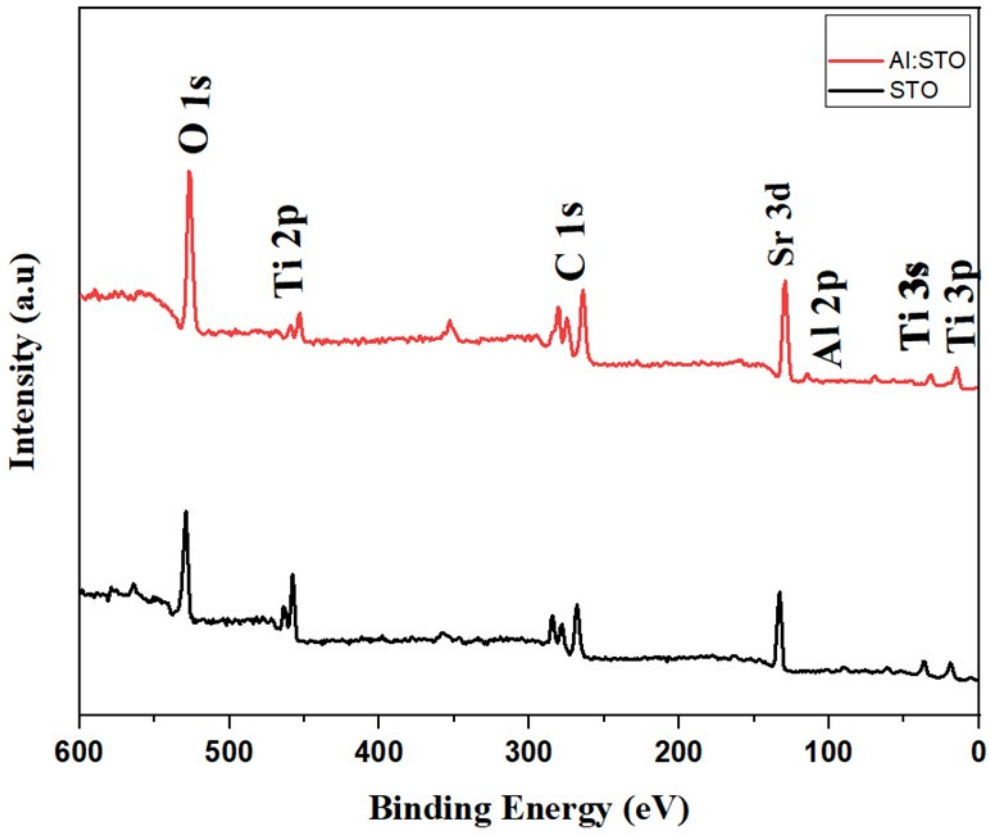

Fig. 3 X-ray photoelectron spectroscopy (XPS) spectra of STO and Al: STO

To study the optical properties of Al: STO Uv-visible and UPS analysis were performed to investigate the energy bandgap and valence band maximum position. Fig. 4(a, b) shows the absorption spectra of Al: STO before and after performance signifying that bandgap got reduced after performance leading to enhance the charge transport at the interface via the induced intermediate states. Moreover, UPS analysis were performed to elucidate the valence band position of Al: STO before and after testing as demonstrated in Fig. 4(c, d). The obtained valence band value and bandgap values were used to inculcate the conduction band to construct the energy band diagram to study the charge transport at the interface [2].

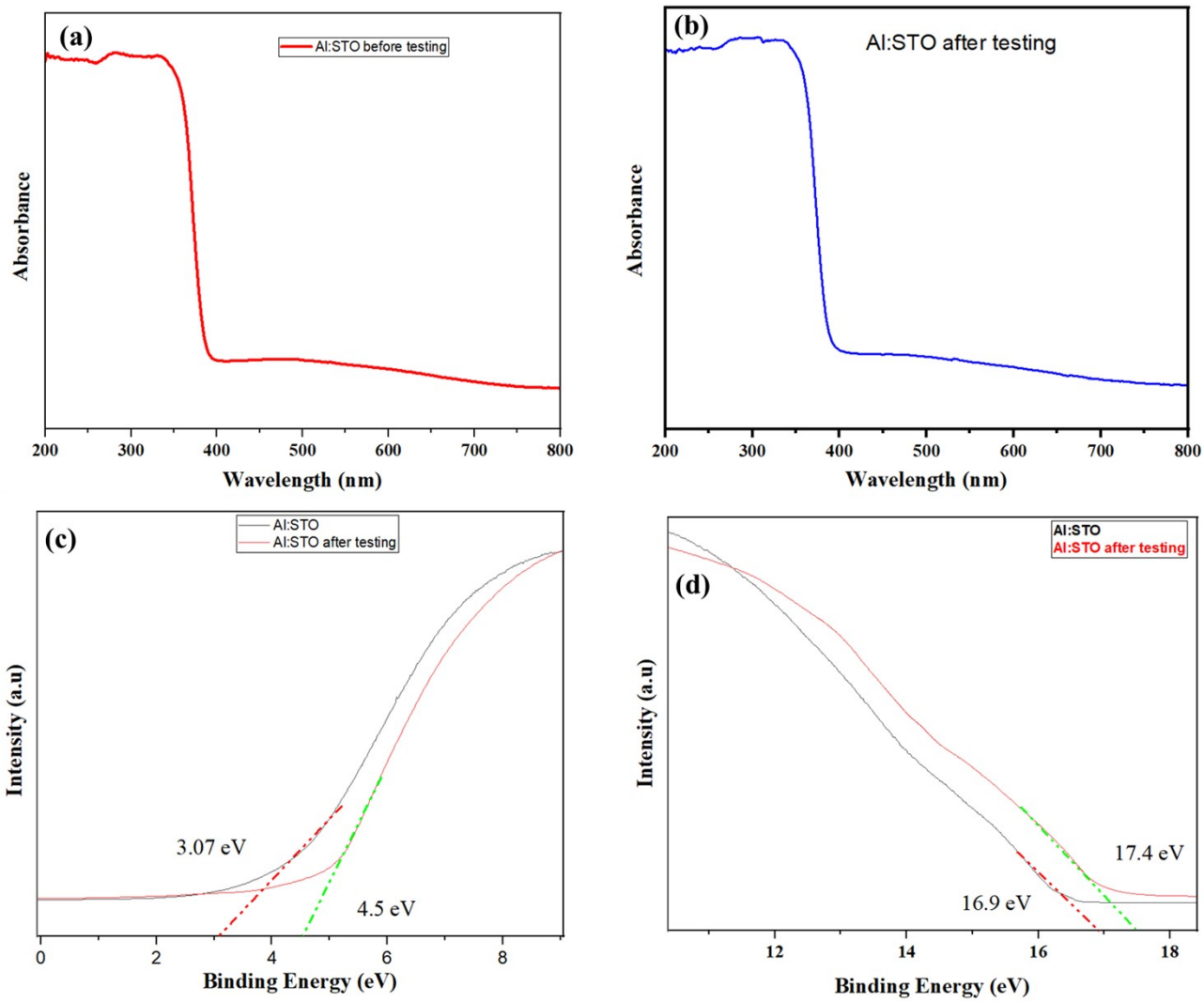

Fig. 4 (a, b) Uv-visible absorption spectra of Al: STO before and after testing while, (c,d) reveals the UPS spectra of Al: STO before and after testing

References

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